Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 137 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.12e-01

Confidence level: 7.52e-01

Nearest Neighbors from the Training Set

Image not found
Aminopropionitrile
Measured: 213
Predicted: 1.81e-01

Image not found
Methyldichlorosilane
Measured: 140
Predicted: 345

Image not found
5-Nonanone
Measured: 178
Predicted: 6.96e-01

Image not found
Trichlorofluoromethane
Measured: 16.7
Predicted: 651

Image not found
Bromotrifluoromethane
Measured: 40.7
Predicted: 6290